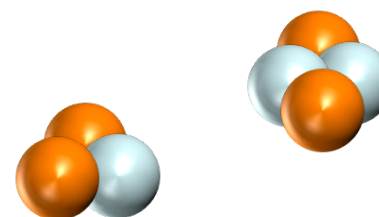
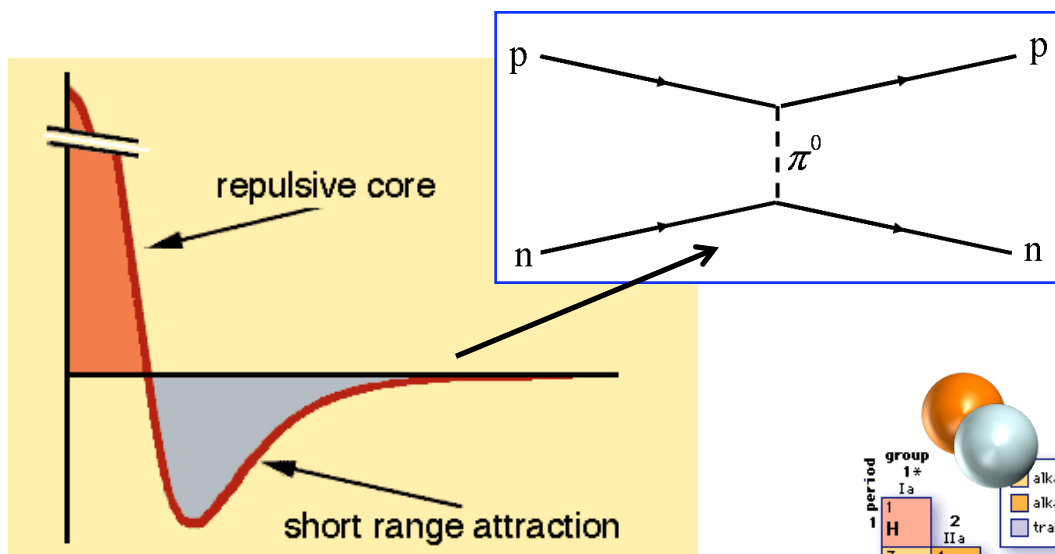


Nuclear Forces and High-Performance Computing: The Perfect Match

June 18, 2009

Tom Luu

The Nuclear Force 101...



The nuclear force is responsible in forming self-bound systems of neutrons and protons, i.e. nuclei and their isotopes

group	1*	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Ia	IIa	IIIa**	IVa	Va	VIa	VIIa	VIIIa	VIIIb	IXa	Xa	IB	IIB	IIIB	IVb	Vb	VIb	VIIb	VIIIb
1	H	He											B	C	N	O	F	Ne
2	Li	Be											Al	Si	P	S	Cl	Ar
3	Na	Mg	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	Ac															
			58	59	60	61	62	63	64	65	66	67	68	69	70	71		
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
			90	91	92	93	94	95	96	97	98	99	100	101	102	103		
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		

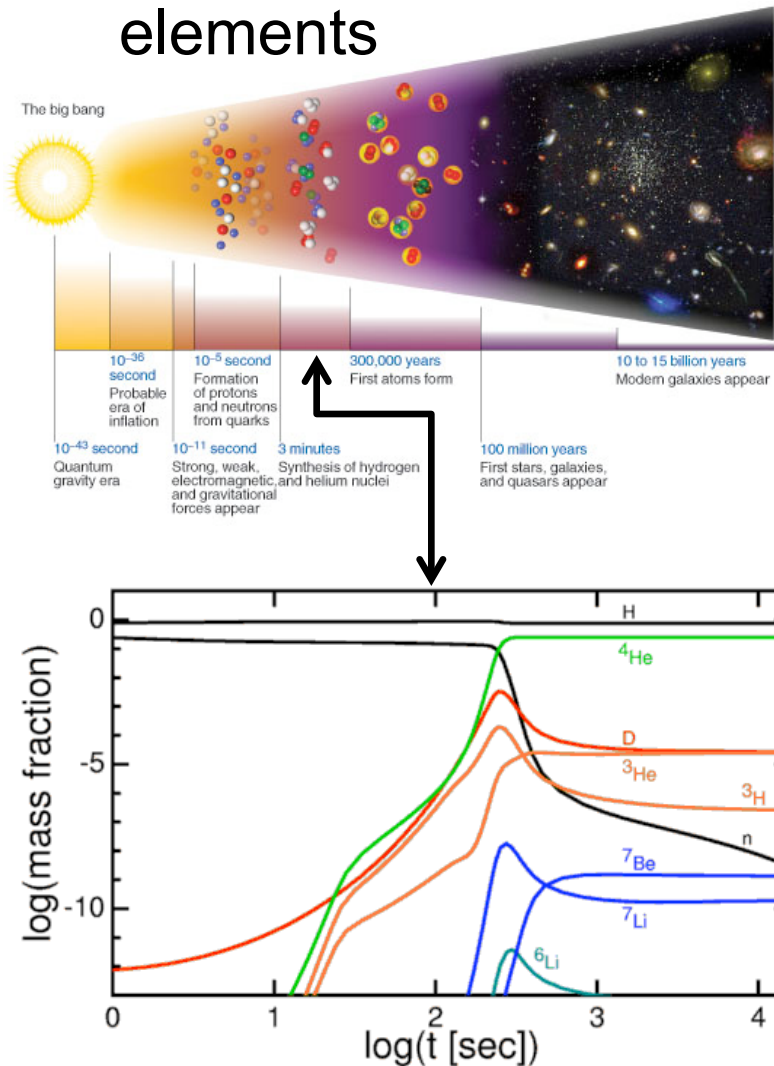
* Numbering system recommended by the International Union of Pure and Applied Chemistry (IUPAC)
 ** Previous IUPAC numbering system
 *** Numbering system recommended by the Chemical Abstracts Service
 **** For the names of elements 104–112, see Table 27.

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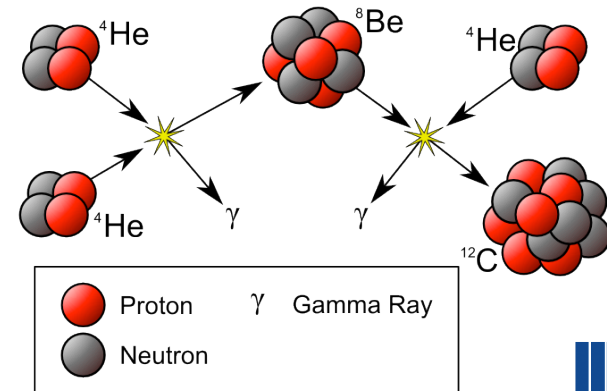
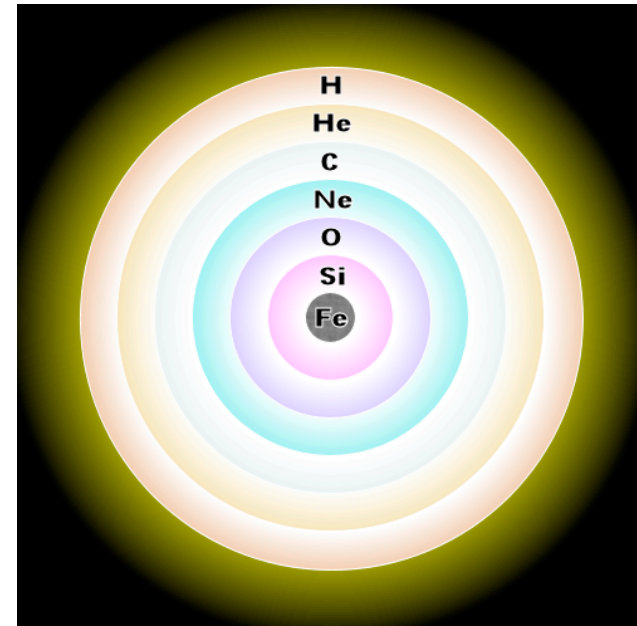


The nuclear force plays an integral role in the evolution of our universe. . .

■ Synthesis of primordial elements

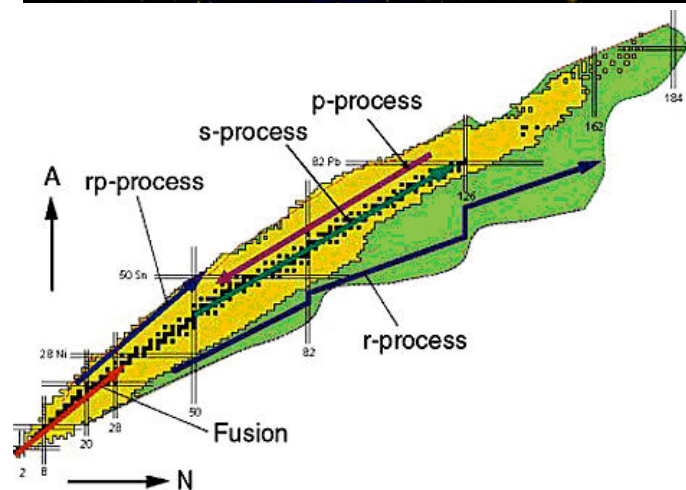
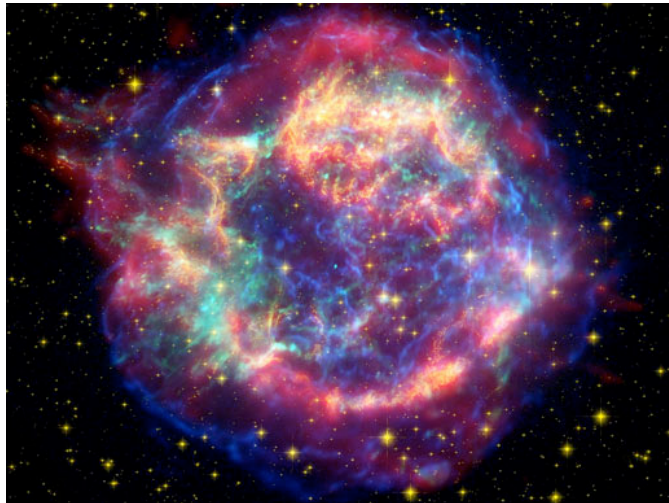


■ Fusion in stars

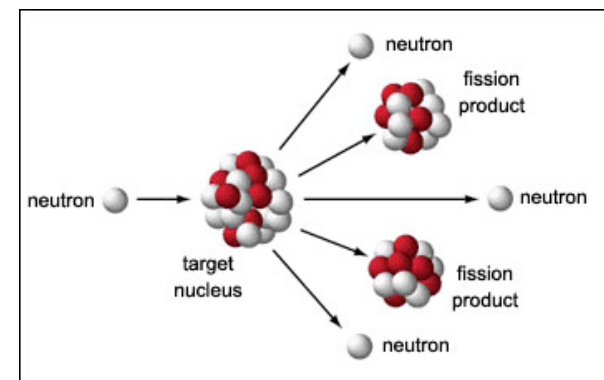
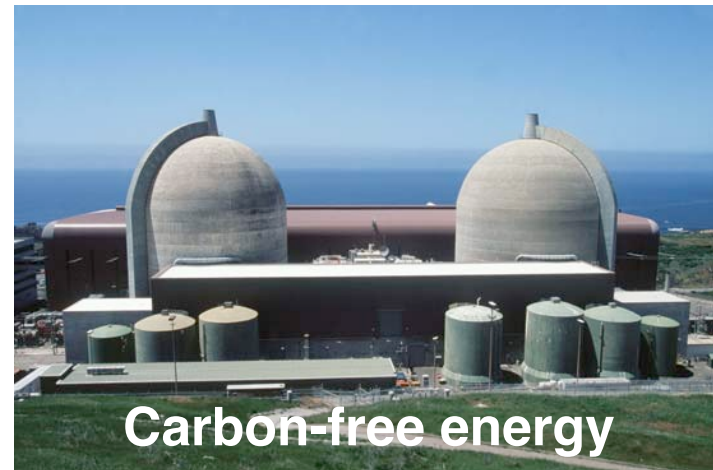


... and is responsible for a diverse range of physical phenomena

- Responsible for 'core-bounce' in supernovae

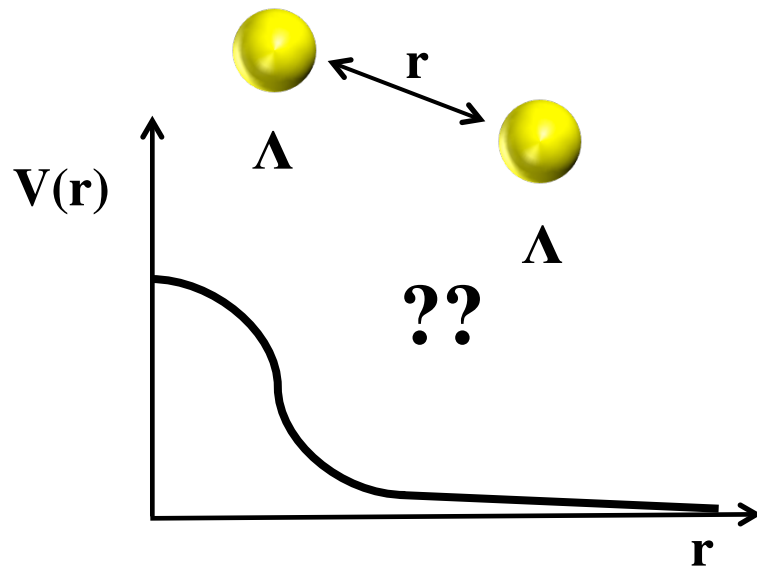


- Fission

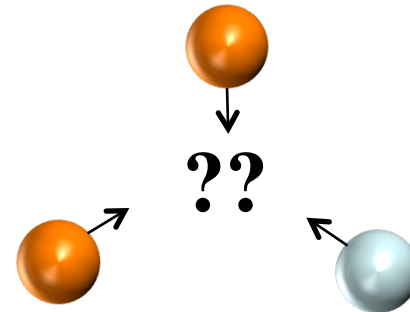


However, there are aspects of the nuclear force that are poorly understood even today. . .

- What is the force between two hyperons?



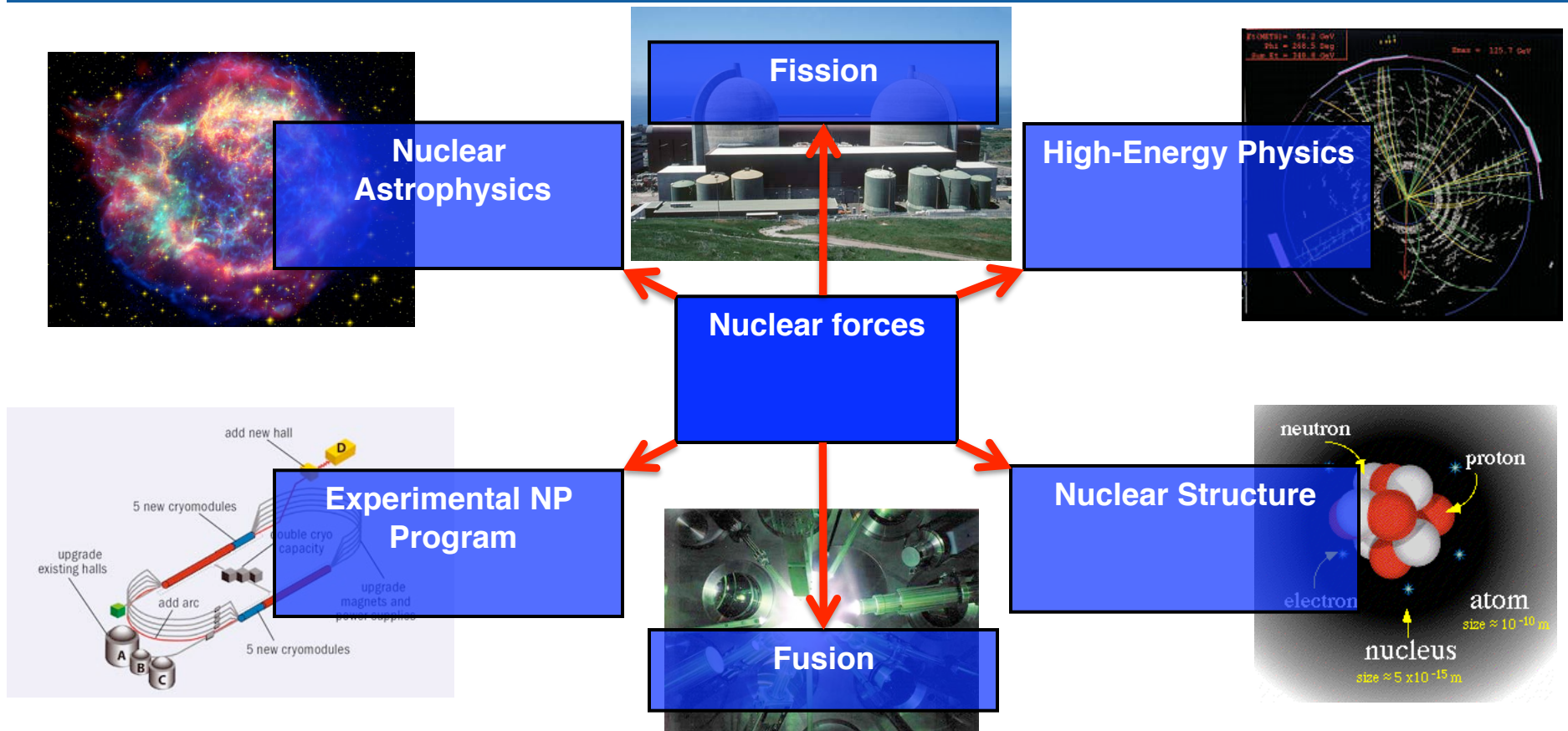
- What is exact nature of 3-body forces in nuclear physics?



And the list of questions goes on and on . . .



Answers to many of these questions have implications to the broader physics community. . .

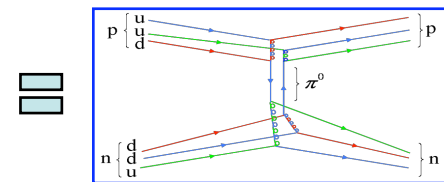
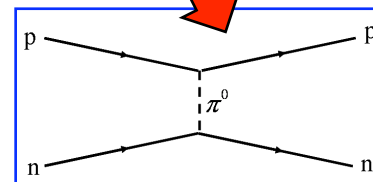
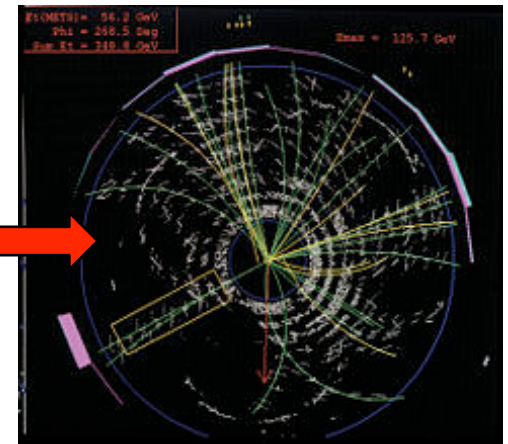
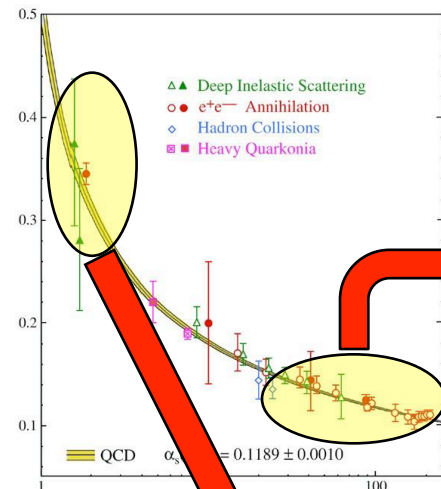
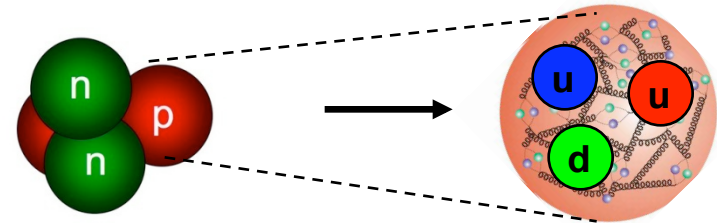


*Nuclear forces plays a key role
in many fields of physics*



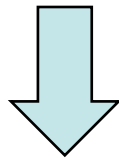
So why can't we answer these questions?

- The nuclear force is not fundamental
 - Governed by the underlying theory of quarks and gluons —QCD
- At high energies ($\gg 1$ GeV), theory exhibits 'asymptotic freedom'
 - In this regime, QCD has been well tested perturbatively
- At low energies (< 1 GeV) QCD is a strongly-interacting theory
 - We have no formal (paper & pencil) way of solving QCD in this regime

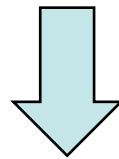


QCD is exceptionally hard to calculate in the low-energy regime!!!

Feynman's path integral
formulation accounts for
quantum fluctuations

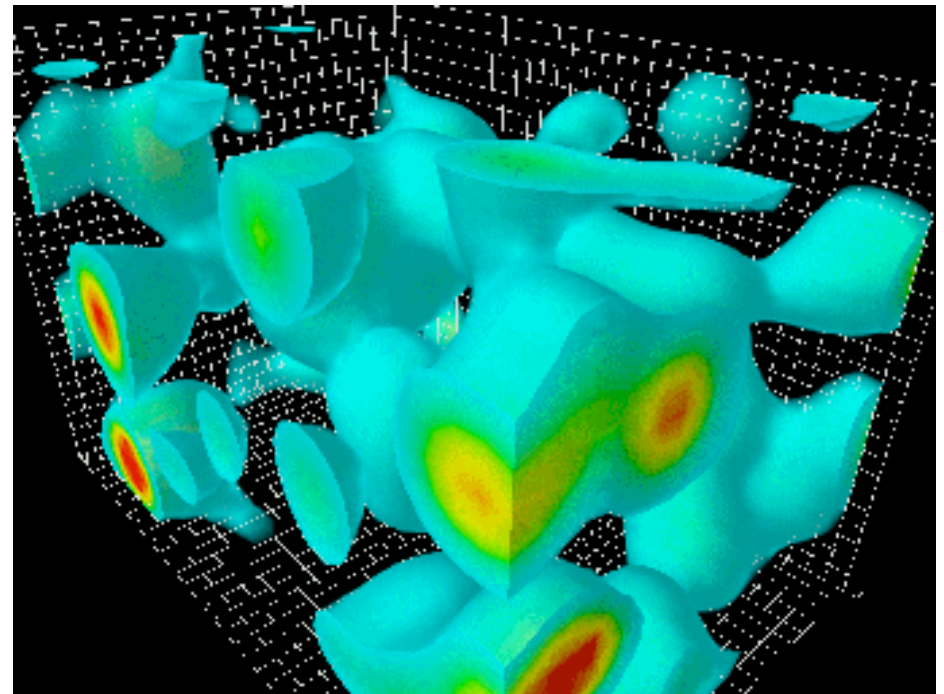


Sum over all possible paths

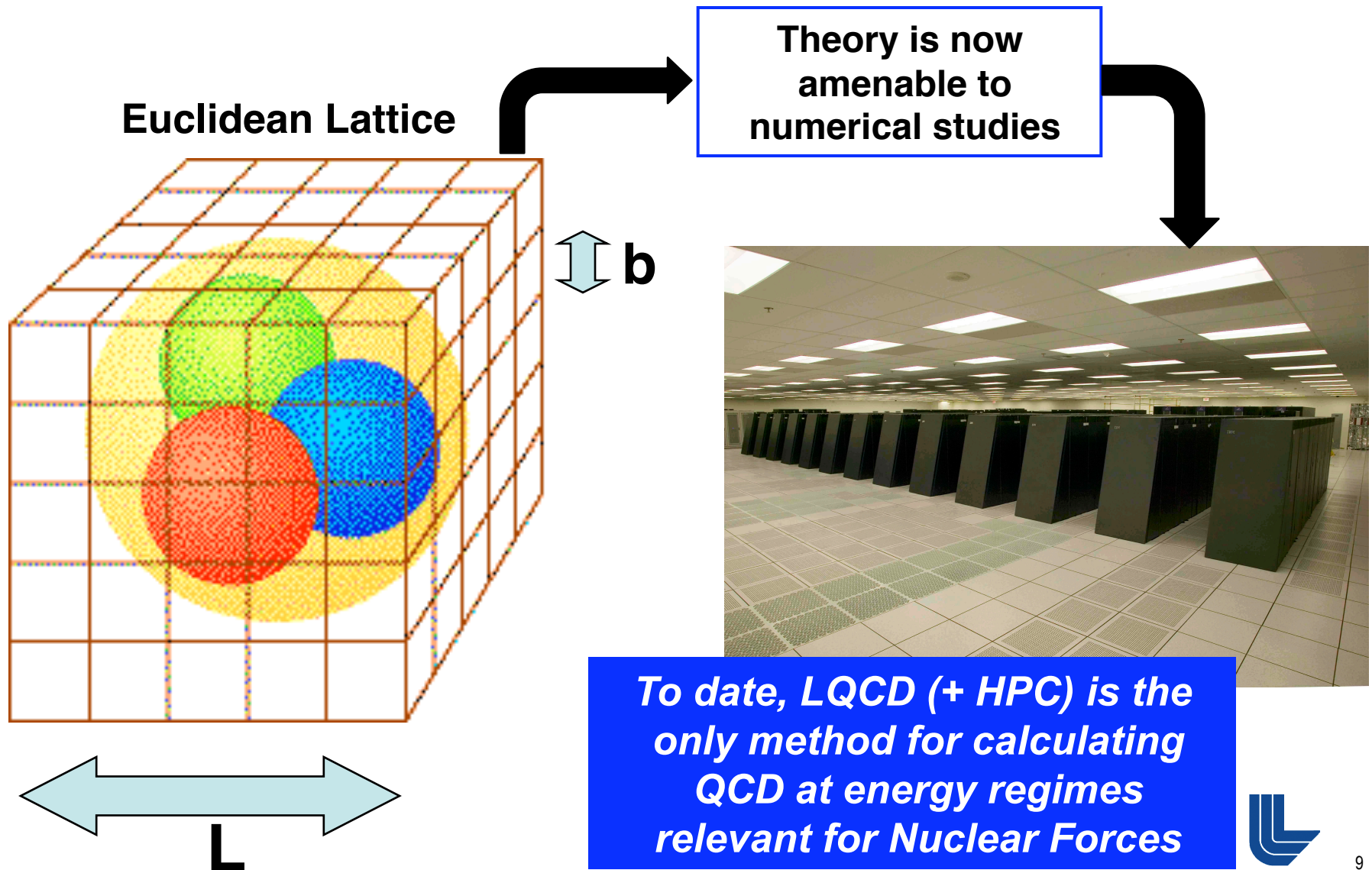


Infinite-dimensional integral!

Quantum fluctuations



So let's put an "L" in front of QCD

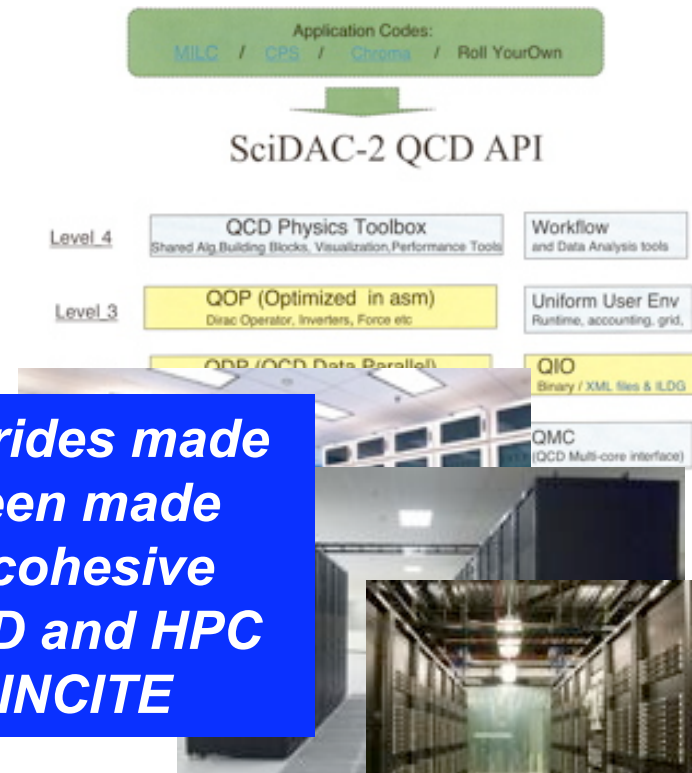


- SciDAC support for development and maintenance of LQCD codes

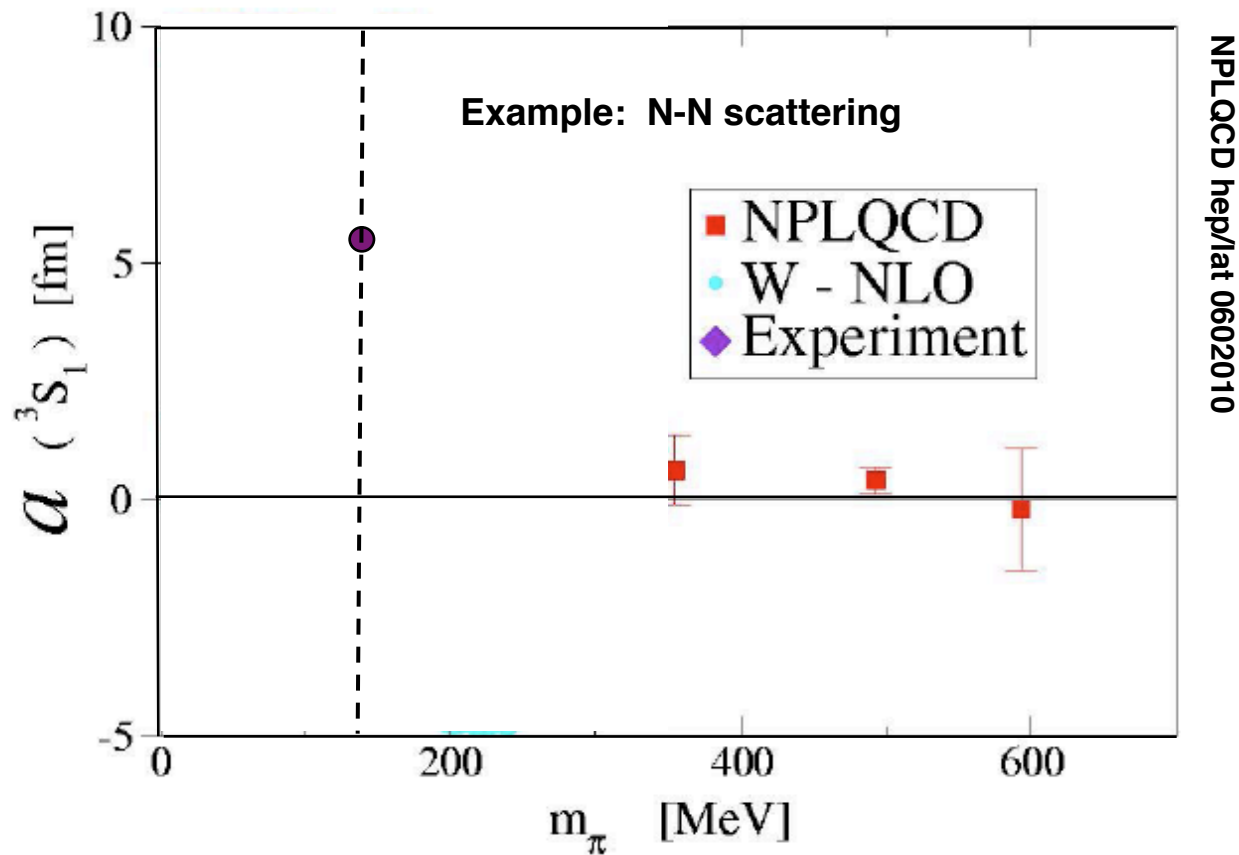
- DOE support and acquisition

The recent large strides made in LQCD have been made possible by the cohesive program of USQCD and HPC allocations by INCITE

- Allocations given through DOE's INCITE program



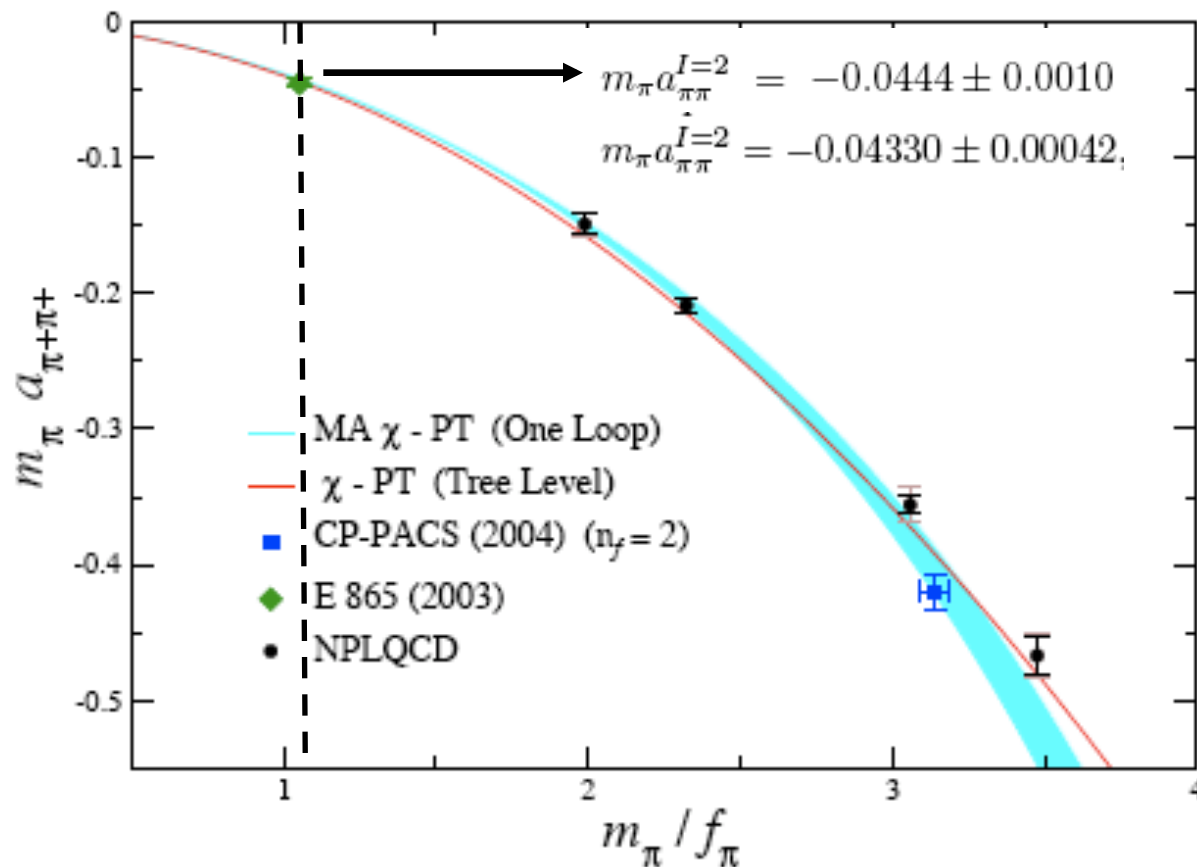
The Nuclear force is perturbative at larger-than-physical pion mass



High-performance computing is allowing us to understand how nature depends on fundamental constants of nature



Weinberg's prediction for the interaction between pions works surprisingly well



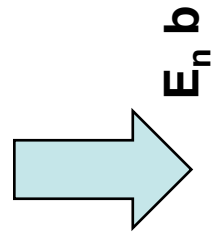
Pislak et al. hep/ex
0301040

NPLQCD hep/lat
0706.3026

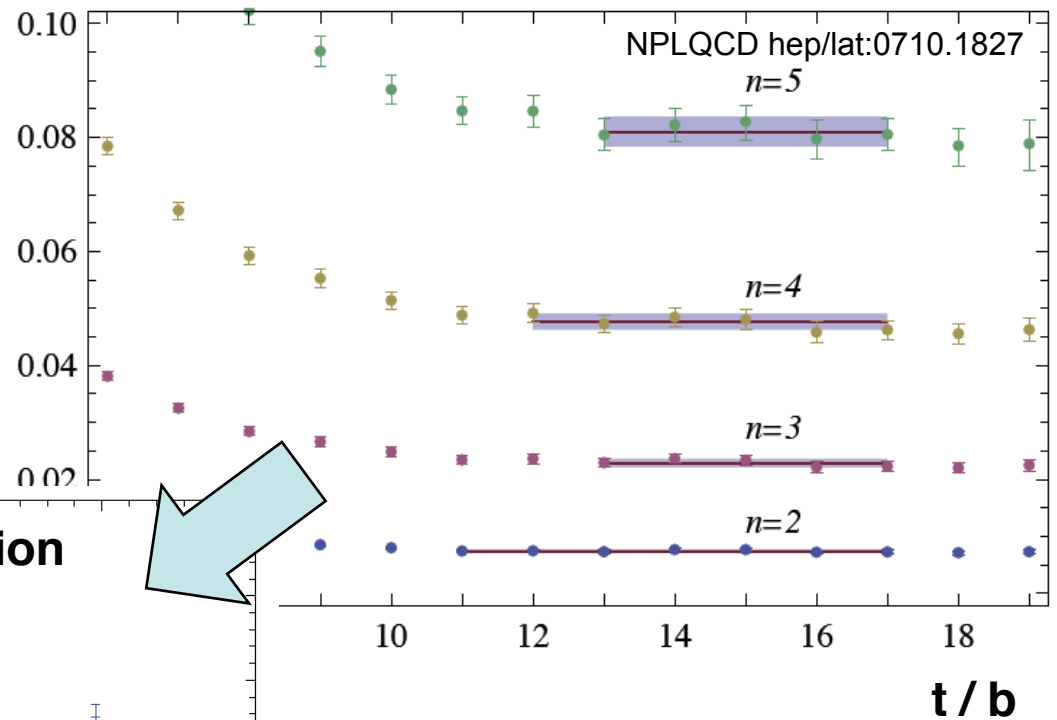
In certain cases, HPC (+ LQCD) is allowing precision calculation of nuclear forces at the sub-percent level

We now know pions have a repulsive three-body force

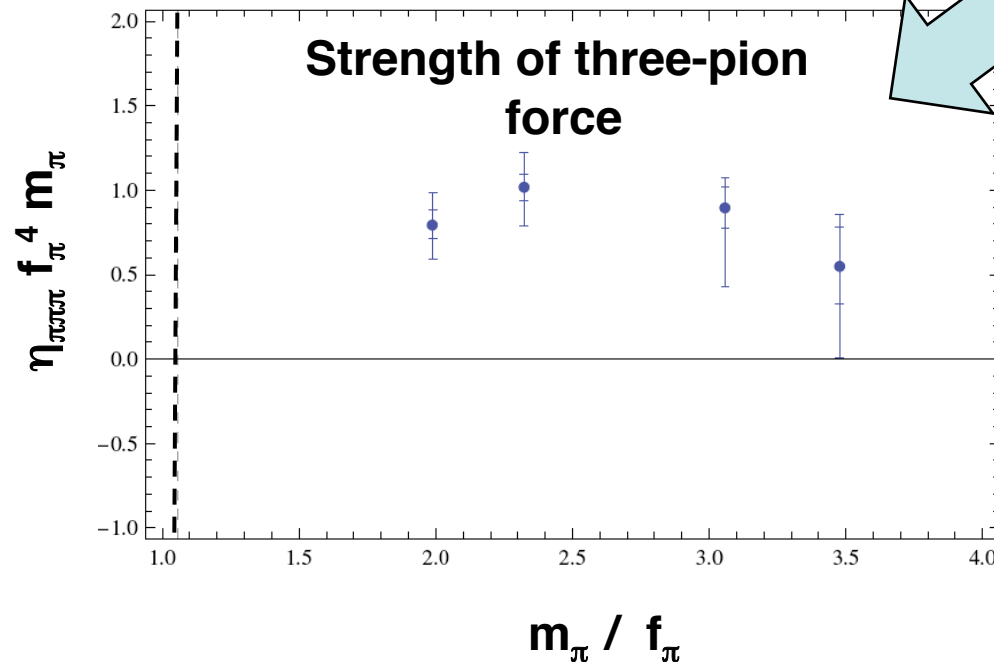
The interaction energies of multiple pions in a box



$E_n b$



Strength of three-pion force

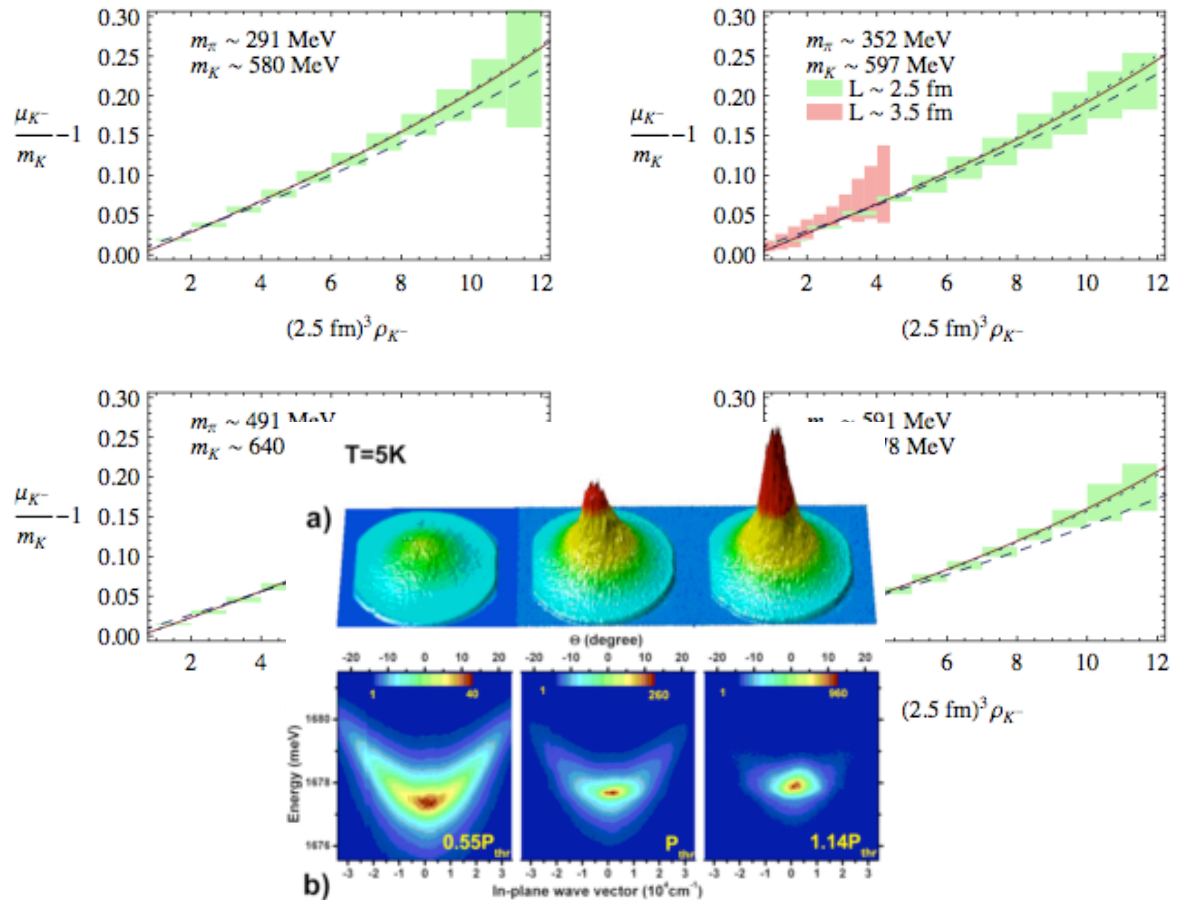


High-performance computing is allowing us to probe systems that are experimentally inaccessible

Kaon condensation—simulating a Bose-Einstein Condensate

**Kaon chemical
potential as a
function of number
density**

**Rubidium atoms
in an atomic
trap**



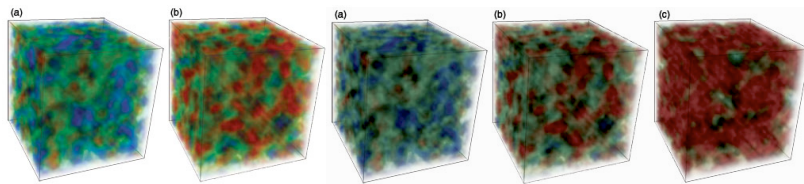
*High-performance computing is
allowing us to solve the quantum
many-body problem*

hep-lat/0807.1856

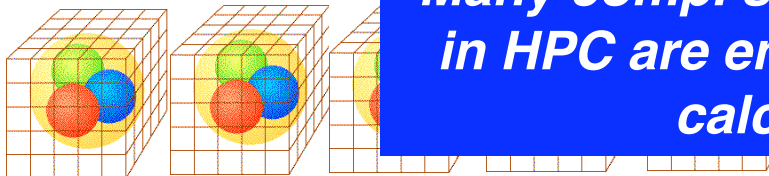


What makes nuclear forces and HPC the perfect match? Part 1)

- Generation of gluon fields



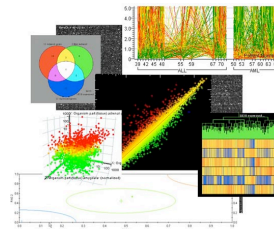
- Measurements



Many comp. sci. and applied math. issues in HPC are encapsulated in nuclear force calculations via LQCD

- Contractions

- Extraction of Observable



- Hybrid Monte Carlo

- Molecular dynamics integrator (e.g. Omelyan)
- Sparse matrix inversion (e.g. CG, CG+deflation, BCGStab)
 - Condition number $\sim 10^{7-8}$
- Problem scales as $b^{-6} L^5 m_\pi^{-3}$

- Forming physically relevant objects

- Combinatoric—essentially serially so far

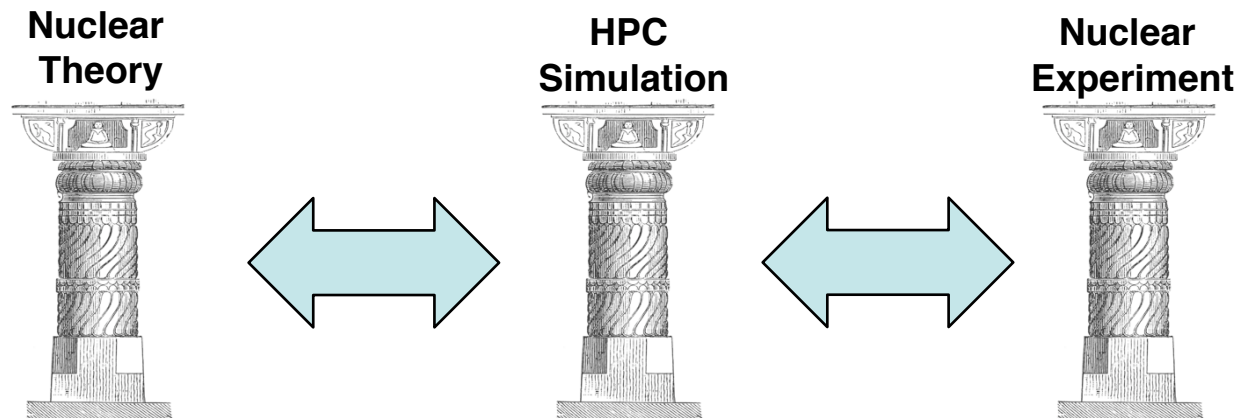
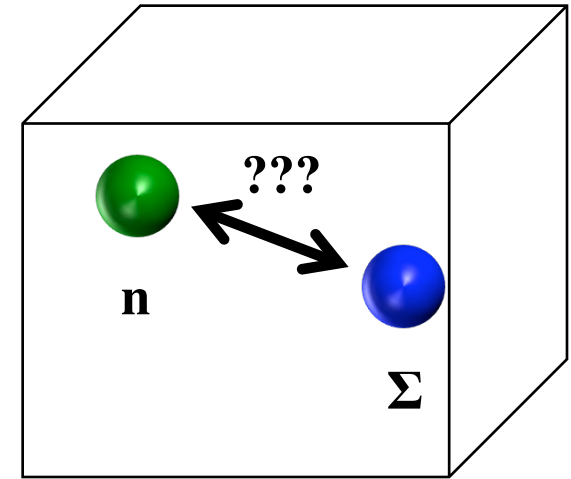
- Data Analysis

- Large ‘noisy’ data sets
- Dispersed on different machines

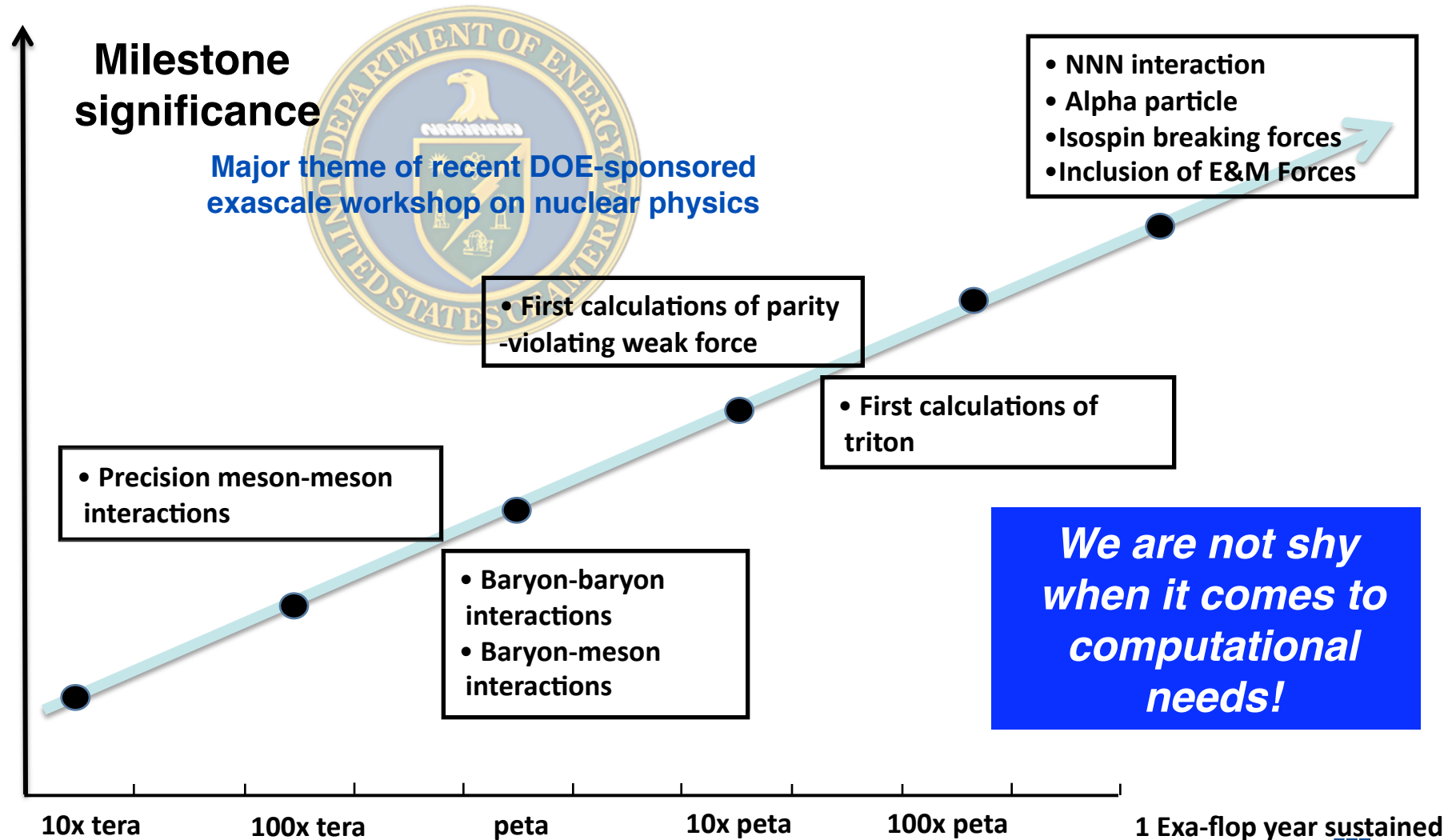


What makes nuclear forces and HPC the perfect match? Part 2)

- Example: What is the interaction between a neutron and sigma?
- Experimentally inaccessible
- HPC + LQCD can calculate the interaction terms
- HPC + LQCD can guide future experimental efforts



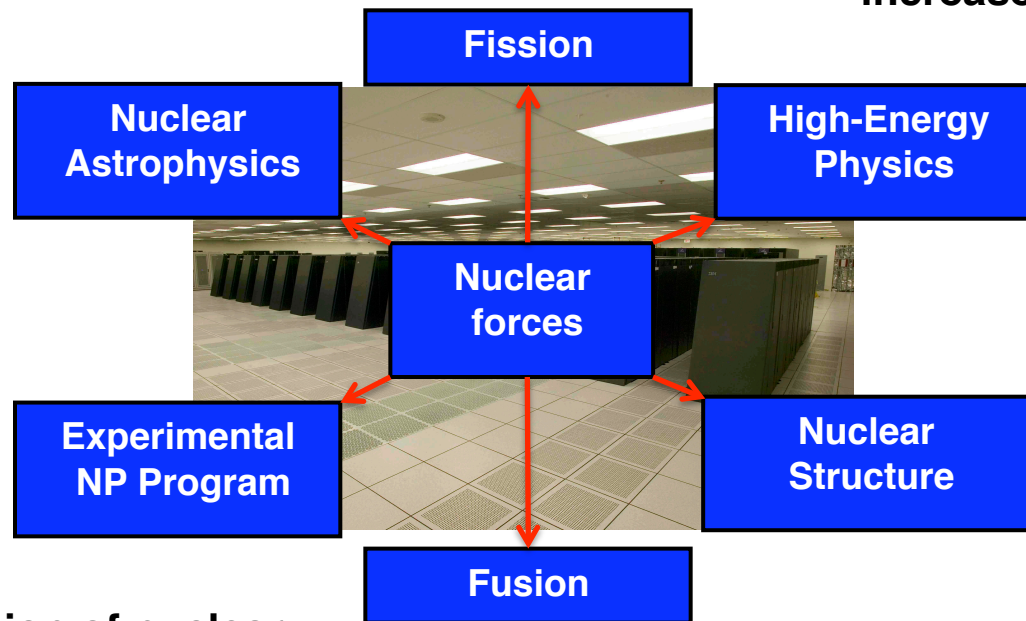
Milestones in calculating Nuclear Forces from QCD . . .



The future of HPC and Nuclear Physics

Lattice QCD will become a powerful calculational tool available for nuclear scientists

The various subfields of nuclear physics will operate with increased synergism



The next generation of nuclear scientists will be experts in both HPC fields and nuclear physics

Predictive capability will become the norm in nuclear science



The Unification of Nuclear Physics due to High-Performance Computing

